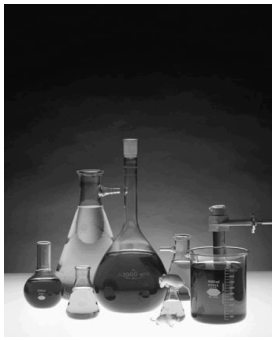

Determination of Chemical Formulas

- **molecular formulas** - numbers of atoms of each element in a molecule
- **empirical formulas** - relative numbers of atoms of each element using the smallest whole numbers

Example:

acetic acid → $C_2H_4O_2$ (MF) → CH_2O (EF)
formaldehyde → CH_2O (MF) → CH_2O (EF)
glucose → $C_6H_{12}O_6$ (MF) → CH_2O (EF)

- Conversion between masses of compounds and masses of their elements using chem. formulas

Example: What is the mass of H in 5.00 g CH_4?

CH_4 → *M* = 1×12.01 + 4×1.008 = 16.04 g/mol
H → *M* = 1.008 g/mol

$$5.00\text{ g CH}_4 \times \left(\frac{1\text{ mol CH}_4}{16.04\text{ g CH}_4}\right) \times \left(\frac{4\text{ mol H}}{1\text{ mol CH}_4}\right) \times$$
$$\times \left(\frac{1.008\text{ g H}}{1\text{ mol H}}\right) = 1.26\text{ g H}$$

2.11 Mass Percentage Composition

- Percentage by mass of each element in a compound
- **Mass% = [$m_{element}/m_{compound}$]×100%**

- Calculation of Mass% from chemical analysis
- **Example:** Calculate the mass percentage of C in nicotine, if analysis shows that 5.00 g of nicotine contain 3.70 g C, 0.44 g H and 0.86 g N.

$$\text{Mass\% C} = \left(\frac{3.70\text{ g C}}{5.00\text{ g nicotine}}\right) \times 100\% = 74.0\%$$

- Calculation of Mass% from chemical formulas

Example: Calculate the Mass% of O in CO_2.

CO_2 → *M* = 1×12.01 + 2×16.00 = 44.01 g/mol
O → *M* = 16.00 g/mol

Consider: 1 mol CO_2 → contains 2 mol O

→ mass of 1 mol CO_2 = 44.01 g CO_2

→ mass of 2 mol O = 2 mol O×[16.00 g O/1 mol O]= = 32.00 g O

$$\text{Mass\% O} = \left(\frac{32.00\text{ g O}}{44.01\text{ g CO}_2}\right) \times 100\% = 72.71\%$$

2.12 Determining Empirical Formulas

- The relative number of atoms of each element is the same as the relative number of moles of each element in a compound

- EF from Mass% data
  - consider 100 g of the compound
  - the masses of the elements equal their mass%
  - convert the masses of the elements to moles
  - determine the relative number of moles (mole ratio)
  - simplify the mole ratio to whole numbers

Example:

- Determine the EF of nicotine, if the mass% of C, H and N in it are 74.0, 8.7 and 17.3 %, respectively.

→consider 100 g nicotine

→74.0 g C, 8.7 g H, 17.3 g N

→convert masses to moles:

74.0 g C×(1 mol C/12.01 g C) = 6.16 mol C

8.7 g H×(1 mol H/1.008 g H) = 8.6 mol H

17.3 g N×(1 mol N/14.01 g N) = 1.23 mol N

→mol ratio:

6.16 mol C : 8.6 mol H : 1.23 mol N

→simplify the mole ratio:

6.16/1.23 = 5.01 ≅ 5

8.6/1.23 = 7.0 ≅ 7

1.23/1.23 = 1.00 ≅ 1

→simplest whole-number ratio:

5 mol C : 7 mol H : 1 mol N

→EF:

$\mathbf{C_5H_7N}$

2.13 Determining Molecular Formulas

- The MF is a whole-number multiple of the EF

$$\Rightarrow \boldsymbol{M = M_{EF} \times n}$$

  - $\boldsymbol{M}$ → molar mass
  - $\boldsymbol{M_{EF}}$ → EF mass
  - **n** → whole number (number of EFs per molecule)

$$\Rightarrow \mathbf{n = M/M_{EF}}$$

- Determining MFs from EFs and molar masses

Example:

- The empirical formula of nicotine is $\mathbf{C_5H_7N}$ and its molar mass is 162.23 g/mol. MF = ?

$\boldsymbol{M_{EF}}$ **→ 5×12.01+7×1.008+1×14.01 = 81.12 g/mol**

$$n = \frac{M}{M_{EF}} = \frac{162.23\ g/mol}{81.12\ g/mol} = 2.000 \cong 2$$

⇒MF = 2 × EF

MF → $\mathbf{C_{10}H_{14}N_2}$

Assignments:

- **Homework: Chpt. 2**/3, 5, 9, 11, 13, 15, 17, 19, 23, 25, 29, 31, 33, **35, 43, 47, 49, 51, 57, 61, 65, 69, 71, 73, 99.**
- **Student Companion:** 2.1, 2.2, **2.3**